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Modified Charge Bag Model of Superconductivity

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Abstract

The 'Modified Charge Bag' model essentially provides a microscopical derivation of the nested Fermi liquid (NFL) theory. The model has wide range of applicability to non-cuprate high temperature superconductors, including some of the organic superconductors like $(BEDT-TTF)_2I_3$. The model invokes a completely new mechanism of superconductivity based on the strong electron-phonon interaction which explains the expected behaviour of superconducting (SC) transition temperature T_c with the dopant concentration (δ). T_c increases with δ in low-doping regime where as it decreases with δ in higher doping regime. The SC order parameter possesses d-wave like symmetry. However, explicit evaluation of the SC-gap function derived from the SC-gap equation supports anisotropic but s-wave like pairing. The s-wave nature of superconductivity is confirmed, as the SC-gap function carries exactly similar (in-built) symmetry of the original 2-d square lattice.

Keywords: Charge bag model, d-wave superconductivity, nested Fermi Liquid theory.

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1 Introduction.

The whole family of high-T_c superconductors can be broadly classified into two categories namely, the Cuprate High-T_c superconductors and the copperless high-T_c superconductors. The $Cu-O$ high-T_c materials as is realised by now exhibits many many exciting and anamalous normal state properties (i.e, the properties differ from the usual understanding of conventional metals). However, the non-cuprate high-T_c superconductors [e.g, $Ba_{1-x}K_xBiO_3$ ($T_c \sim 32K$), $BaPb_{1-x}Bi_xO_3$ ($T_c \sim 15K$), A_3C_{60} (A=K, Rb) ($T_c \sim 28K$) etc.] along with some of the organic superconductors like $(BEDT-TTF)_2I_3$ (ET) family show similarity in a number of normal state properties with that of the cuprate superconductors. The linear temperature dependence of resistivity ($\rho_{ab} \sim T$), the observation of constant background intensity in the Raman spectrum, the mid gap observation in optical conductivity etc. are few of the anamolous properties common to both cuprates and non-cuprate [1, 2, 3, 4, 5]. Therefore, the normal state properties of the non-cuprate high-T_c superconductors as well as the superconductors like ET-family are equally anamalous and exciting which needs extensive theoretical as well as experimental investigations. Since the phenomenological marginal Fermi Liquid (MFL) theory can explain most of these anamolous properties ;it is expected to look for theories which essentially provide a microscopic derivation of the MFL [6] for aproper understanding of these systems. Nevertheless, since it is believed that it is the strong electron-phonon interaction which predominently controls the essential properties of non-cuprates rather than strong electron correlation as in case of cuprates —-the nested Fermi liquid [7] kind of theory based on weak Coulomb correlation would probably be an appropiate starting point. An attempt in this direction was made by Gaitonde and Behera [8] who proposed the 'charge bag model'. A brief account of thephysical picture of this theory is given in sec.2. In sec.3 we point out the crucial limitations of the above model and describe the essential features of the proposed 'modified charge bag model' which incorporates the neccessary modification over the 'charge bag model'. In this section a brief discussion of symmetry of the order parameter is also presented. Finally we conclude by summarizing the essential results in sec.4.

2 Charge bag model

Although there are similarity in a number of physical properties among the cuprates, non-cuprates and the organic superconductors ($BEDT-TTF$) as mentioned earlier there are essential differences as well. Almost all non-cuprate high-T_C materials along with the ET superconductors are non-magnetic (paramagnetic) in their ground state

(unlike the cuprates which show long range antiferromagnetic ordering) which clearly indicates that the mechanism of superconductivity in the two classes of materials will be of different origin. The undoped normal state of the Bismathate high-T_c superconductors are known to be charge density wave (CDW) insulator (e.g, $Ba_{1-x}K_xBiO_3$ and $BaPb_xBi_{1-x}O_3$ etc. for $x = 0$) [8]. Presence of high degree of nesting in the Fermi surface together with strong electron-phonon interaction destabilizess the normal metallic state and transforms it to the CDW insulator. The idea of the Peierl's transition is that it is always possible to lower the electronic energy of such a system by setting up a CDW of suitable wave length such that the new periodicity will give rise to a brillouin zone boundary resulting in a gap at the Fermi-level and hence the metal will transform into a CDW insulator. In order to metalize this insulator and to build superconducting instability one needs to dope the system with free charge carriers. If the system is doped with holes which essentially means removal of electrons from the lower CDW band the CDW gap will be suppressed locally. The local depression in the CDW gap will act as a potential well for the injected charge carrier in which it will be self-trapped producing the 'charge bag'. This is so because in the process of taking away of electron (hole doping), the net gain in energy that the system acquires in stabilization against the CDW formation will be partially lost. On the other hand, it is energetically favourable for two holes of opposite spins to occupy the same bag digging a deeper well. Such a pairing is equivalent to a cooper pairing that arises because of an effective attractive interaction between the injected carriers mediated by the exchange of the quanta of fluctuation of the amplitude and phase of the CDW gap. This is known as the 'charge bag model' [8] of superconductivity. Even though there is no direct experimental evidence of CDW instability in the normal state of the organic superconductor ET family an incommensurate transition is known to occur in some varriants of the above compound and therefore, the normal state of these can also be modelled as a CDW insulator, and hence the charge bag mechanism can be operative.

3 Modified charge bag model

Although 'charge bag model' can explain qualitatively the mechanism of high-T_c in non-cuprates, the model has a few crucial limitations and needs neccessary modifications. Strictly speaking, the above picture holds good only in the limit of low doping limit simply because in this case the FS will retain its perfect nesting which is needed to keep intact the CDW gap. Secondly, in such a picture the SC-pairing takes place only either in the valence band (for hole doped systems) or in the coduction band (electron doped systems). As a consequence the calculated Raman spectrum does not show the

signature of the CDW gap mode. However, to be realistic, the superconductivity in $Ba_{1-x}K_xBiO_3$ appears only at a rather large doping i.e, $x \geq 0.37$ for). It is expected that at such large dopant concentrations the Fermi surface (FS) will loose its perfect nesting behaviour.

Therefore, we propose that the nesting of the FS will be preserved only upto a certain dopant concentration. Since there are experimental evidences that the signature of the CDW state exists even at very large doping (e.g, for $Ba_{1-x}K_xBiO_3$ at $x = 0.4$) [9] we propose that there will be certain directions in which nesting will be destroyed resulting in the collapse of the CDW gap whereas in certain other directions nested pieces of the FS will still exists resulting in the appearence of the CDW-gapped regions. Hence, the FS is now end up acquiring a pseudo-gap rather than a real and isotropic gap, as discussed in [8]. The more the system is doped the more regions of the FS will be without a gap leaving very small pockets of gapped regions. The gapless regions of the FS is most likely to be a nested fermi liquid [7]. However, the identity of a quasi particle in the gap free region of the FS would be that of either of the conduction or the valence band. Under this scenario, we envisage that the pairing will take place predominently between the CDW quasi particles coming from both the bands mediated by the quanta of fluctuations of the CDW-gap. This is in essence is the 'modified charge bag' model. The existence of stable CDW gapped region of the FS is however essential, because it is the quanta of fluctuations of the CDW gap that mediates the pairing. Detailed microcopics of the model will be published elsewhere [11].

The ground state of the undoped systems are essentially CDW insulators can be be obtained from the metallic state described by the Hamiltonian [8],

$$H = \sum_{k,\sigma} \hat{\Psi}^{\dagger}_{k,\sigma}[(\epsilon_k - \mu)\hat{\tau}_3 + W\hat{\tau}_1]\hat{\Psi}_{k,\sigma} \tag{1}$$

where $\hat{\Psi}^{\dagger}_{k,\sigma} = (C^{\dagger}_{k,\sigma} \quad C^{\dagger}_{k+Q,\sigma})$ is a two component Nambu operator and τ_i's are the Pauli matrices. Where W is the CDW order parameter given by,

$$W \equiv -V \sum_{k,\sigma} < C^{\dagger}_{k+Q\sigma} C_{k\sigma} >= -V < \rho_Q > \equiv g < A_Q > \tag{2}$$

which is nothing but proportional to the $Q - th$ component of the electronic charge density and V is the strength of the attractive effective electron-electron interaction. On the other hand, the formation of the CDW will be coupled with the periodic lattice distortion of the underlying lattice. Therefore, the CDW state can equivalently be obtained assuming the amplitude of the Q-th mode of the phonon to be constant (as is given in the last term of eqn.(2)).

Doping over the CDW state essentially creates fluctuations over the stable CDW

state which can be described from (2) as,

$$W + \tilde{W}_{iq} \equiv g[< A_Q > + (\tilde{b}^i_q + \tilde{b}^{i\dagger}_{-q})] \tag{3}$$

where $\tilde{W}_{iq}$ corresponds to the amplitude ($i = 1$) and phase ($i = 2$) fluctuations of the CDW gap the quanta of which are treated as phonons. Therefore, combining equations (1 - 3) one can find the interacting Hamiltonian for the normal state that describes coupling of the CDW quasi particles with the fluctuations of the gap as,

$$\tilde{H}_{e-ph} = g \sum_{i=1,2} \sum_{k,k',q} \hat{\Psi}^{\dagger}_{k+q,\sigma} \hat{\sigma}_i \hat{\Psi}_{k,\sigma} (\tilde{b}^i_q + \tilde{b}^{i\dagger}_{-q}). \tag{4}$$

Equation (4) describes a new kind of electron phonon interaction analogous to Balseiro-Falicov interaction [10] which is responsible for superconductivity in the present mechanism. It is possible to eliminate the phonon degrees of freedom from (4) by usual second order perturbation theory to yield an effective interaction between the CDW quasiparticles in the gap free regions of the FS which could be attractive under appropiate condition giving rise to superconductivity [11].

Since superconductivity appears only in the gapless regions of the FS and as the gapless regions of the FS extends more and more with doping (giving rise to more and more quasi particles to pair up), it is expected that the SC-gap will be an anisotropic one and the T_c will increase with increasing doping (δ) as well as with decreasing W. Therefore, the T_c will increase with δ in low doping regime whereas it will decrease in the large doping limit. We obtain,

$$K_B T_c = 1.13 \Omega_{AM} \begin{cases} \exp(-\frac{1}{(\lambda_1 - \lambda_2)N(0)} + \frac{\lambda_2 N \delta^2}{4W^2 N(0)}); & \textit{for low doping} \\ \exp(-\frac{1}{(\lambda_1 + \lambda_2)N(0)}); & \textit{for large doping} \end{cases} \tag{5}$$

where $\Omega_{AM} = 2W$, the amplitude mode of the CDW state and λ_i's are dimension less coupling constants.

The anisotropic SC-order parameter $\Delta_{SC}(k)$ is defined as,

$$\Delta_{SC}(k) = -\sum_{k'} [\lambda \sin^2(\phi_k + \phi_{k'}) + \lambda' \cos^2(\phi_k + \phi_{k'})] < \gamma^c_{k'\downarrow} \gamma^v_{k'\uparrow} > \tag{6}$$

which is assumed to be real and is invariant under the transformation $v \longleftrightarrow c$. In eqn. (6) $\gamma^{c(v)}_{k,\sigma}$ corresponds to the CDW quasiparticle in conduction (valence) band and $\cos(sin)\phi_k$ are the coherence factors from the CDW state, $\lambda'(\lambda) = (\lambda_1 \pm \lambda_2)/2$ being the dimensionless coupling constants. Interestingly, the SC-gap parameter has d-wave like symmetry under the transformation $k \rightarrow k + Q$ i.e, $\Delta_{SC}(k) = -\Delta_{SC}(k + Q)$. This is so because of the antiperiodic nature of the basis states i.e, $\gamma^c_{k,\sigma} = \gamma^c_{k+Q,\sigma}$ whereas $\gamma^v_{k,\sigma} = -\gamma^v_{k+Q,\sigma}$. Therefore, apparently the d-wave nature of the SC-pairing in the

'modified charge bag' mechanism is prominent. However, the nature of SC-pairing strictly depends on the nature and the shape of the FS. Mere change in the sign of the order parameter need not lead to the conclusion that the pair -ing is d-wave like. We explicit ly calculate the correlation fun -ction given in (6) in the SC-st ate to find the SC-gap equati- -on, the detailed results of whi ch will be published else-where [?] However, the behaviour of the anisotropic-SC gap function is shown in fig1. It clearly show -s that $\Delta_{SC}(k)$ is anisotropic but s-wave like simply because it has always a non-zero value and never changes its sign.The $\Delta_{SC}(k)$ has minimum value at the Fermi- level coresponding to $\epsilon_k = 0$ and the magnitude of the gap shows k -dependence on either side of the Fermi level. The shift of Fermi level with chemical potential (μ) and hence with dop- ing (δ) is reflected when the symmetric SC-gap becomes assymmetric about the Fermi level. All the above features indicate that the gap function has an in-built symmetry of the underlying original lattice. The loss of symmetry of $\Delta_{SC}(k)$ about the fermi level with doping is analogous to the destruction of the nesting property of the original 2-d square lattice FS. Therefore, the SC-gap is strictly s-wave like.

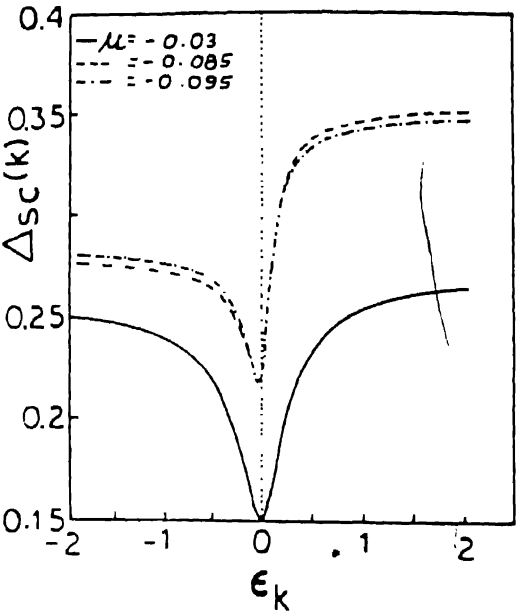

Fig1. The SC-gap function is plotted as a function of ϵ_k for different $\mu(\delta)$ (in arb. units).

4 Conclusion

The 'modified charge bag model' provides a microscopic mechanism of high temperatue superconductivity for the non-cuprates. The essential features of the model emphasising its similarity with nested fermi liquid theory [7] has been explaied qualitatively in detail. A calculation of the Raman Scattering cross-section based on the model sucessfully reproduces the qualitative features of the observed Raman data for the or-

ganic superconductor $(BEDT-TTF)_2I_3$ [12, 13]. The most remarkable feature of the model is that it provides a direct indication of s-wave like anisotropic SC-pairing. The SC-gap function shows s-wave like behaviour even though the order parameter has d-wave like symmetry, which is in-built into the model without any assumptions regarding the k-dependence of the coupling constants. Moreover, it can provide a qualitative explaination of the anamolous normal state properties such as linear temperature dependence of resistivity etc. similar to the MFL.

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